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Scientific Report No. 10 Contract No. AF19(604)-7316 August 1962

SAD NO.

Electron Straggling
Theory and Calculation

by

Nathan Grier Parke III

Project 4608 Task 460802

Electronic Material Sciences
Electronics Research Directorate
Air Force Cambridge Research Laboratories
Office of Aerospace Research
United States Air Force
Bedford, Massachusetts

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Electron Straggling
Theory and Calculation

Nathan Grier Parke III

Introduction.

In the course experimental work on the effect of the passage electrons through a foil on its resistivity, this laboratory undertook some routine calculations of the distribution of the electron energy losses about the mean at different depths in the foil. The initial reference used was "The Passage of Fast Electrons Through Matter; by R. D. Birkhoff, in Volume XXXIV of the Encyclopedia of Physics, Springer, Berlin 1958 pp. 53-138. This starting point quickly lead to the classic paper of L. Landau; J. Phys. USSR, 8 201 (1944) and a paper by T. Blunck and S. Leisegang; Z. Physik 128 500 (1950). We had some difficulties making a calculation that had sufficient validity and avoided enough complications to be useful and tractable. A report of the technical details of this work seems justified.

Importance of Landau's Theory.

A discussion of Landau's paper and theory is important because of the role it plays in the subsequent Blunck and Leisegang work and in the Birkhoff article in the current edition of the massive Handbuch of Physics, edited by S. Flugge and published by Springer, Berlin. In addition, there is an article by Wolfgang Börsch-Supan: "On the Evaluation of the Function

(1)
$$\phi(\lambda) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} u \ln u + \lambda u \, du$$

for Real Values of λ ," Journal of Research of the National Bureau of Standards - B. Mathematics and Mathematical Physics, 65B 245-250 (1961). This function $\Phi(\lambda)$ is Landau's "universal function", describing the transformation of the spectrical distribution of energy. It is the function that was first calculated numerically by the calculation Bureau of the Mathematical Institute of the Academy of Sciences of the USSR. The Börsch-Supan paper presents a table of the function $\Phi(\lambda)$ to five significant figures covering the λ range: -4 (0.025) 4.8 (0.1) 20 (0.2)50(0.5)163. Blünck and Leisegang base their work on a \pm 2% approximation of the Russian calculations as the sum of four Gaussian distributions, i.e.,

(2)
$$\phi(\lambda) = \sum_{i} C_{i} \exp \left[-\left(\frac{\lambda - \lambda_{i}}{k_{i}}\right)^{2}\right]$$

with coefficients:

~	1	2	3	4
c,	0.174	0.058	0.019	0.007
λ	0.0	3.0	6.5	11.0
44	1.8	2.0	3.0	5.0

valid over the range $-2 < \lambda < 15$, with an error of +2%.

By "straggling" is meant the variation in the amount of energy lost by successive particles passing through the medium. To calculate the straggling, is, in theoretical terms, to find the probability density $f(x,\Delta)$ of energy loss Δ after the electron has traveled a distance x in the medium. Landau's solution $f(x,\Delta)$ is related to his universal function $\Phi(x)$ in the following way

(3)
$$f(x, \nabla) = \frac{\beta}{\phi(x)}$$

where,

$$\lambda = \Delta - \frac{1}{5} \left(\ln \frac{\xi}{\epsilon'} + 1 - C \right)$$

$$\ln \epsilon' = \ln \frac{\left(1 - \frac{r^2}{C^2}\right) I^2}{2mv^2} + \frac{v^2}{c^2}$$

$$I_0 = 13.5 \text{ eV}$$
, an ionization potential.

A Discussion of the Landau Theory.

Landau bases his solution on differential-integral equation.

(4)
$$\frac{\partial x}{\partial f(x,\Delta)} = \int_{-\infty}^{\infty} W(\varepsilon) \left[f(x,\Delta-\varepsilon) - f(x,\Delta) \right] d\varepsilon$$

where $W(\xi) = W(\xi_0, \xi)$ is characterized as the probability (per unit length of path) of an energy loss ξ for a particle of energy ξ_0 , where the ionization losses are considered to be small compared with ξ_0 . For W(t) he takes,

(5)
$$W(\varepsilon) = \frac{\pi \operatorname{Ng} e^{4} \sum Z}{\operatorname{mu}^{2} \sum A} \frac{1}{\varepsilon^{2}}$$

where.

N .=. Avogadro's number

m .=. mass of electron

e .=. charge of electron

V .=. related to E_0 by $E_0 = \frac{mv^2}{2}$

? .=. density of substance

ZZ .=. sum of the atomic numbers of the molecules in the substance

A .=. sum of the atomic weights.

The reasons given for equations (4) and (5) left the writer with an uneasy feeling and an attempt was made to find a more satisfactory derivation. One specific cause of uneasiness is the fact that the classical probability density for energy loss & "per collision" is at 1/2 in fact

(6)
$$W_{1}(\xi) = \begin{cases} \frac{\xi_{1}\xi_{2}}{\xi_{2}-\xi_{1}} \cdot \frac{1}{\xi^{2}} & \text{for } \xi_{1} \leq \xi \leq \xi_{2} \\ 0 & \text{otherwise} \end{cases}$$

If there are no collisions per unit distance, and

$$\xi^* = \xi_1 + \xi_2 + \cdots + \xi_{n_0}$$

is the random sum of the energy losses in these no collissions, the the energy loss per unit distance and

(8)
$$W(\xi^*) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{+is\xi^*} \left[\frac{\xi_1 \xi_2}{\xi_2 - \xi_1} \right] \frac{e^{-is\xi}}{\xi_2} d\xi ds$$

is the distribution of the ℓ^* instead of (). The only conclusion one can reach; knowing Landau's stature and ability, is that his results are correct to the order of accuracy he has in mind but their justification can be stated less elliptically. This can be done if we derive equation (4) "collision by collision" rather than "per unit distance".

To begin with let us compute the distribution function

$$f(n+1, \Delta)$$
 .=. probability density for energy loss Δ after $n+1$ collisions

as a function of

 $f(n, \Delta)$.=. probability density for energy loss Δ after n collisions

It is clear that

(9)
$$f(n+1, \Delta) = \int_{0}^{\infty} W_{1}(z) f(n, \Delta-z) dz$$

and hence that the finite difference

$$\frac{\partial f(n,\Delta)}{\partial n} = \frac{f(n+1,\Delta) - f(n,\Delta)}{1} = \int_{0}^{\infty} W_{1}(\xi) \left[f(n,\Delta-\xi) - f(n,\Delta) \right] d\xi$$

If we write

$$\overline{f}(x,\Delta) = f(n_0x,\Delta)$$

WHELE

 n_o .=. average collisions per unit length $n = n_o x$.=. collisions in length x

then

(10,1)
$$\frac{3x}{3\underline{f}(x^{\prime}\nabla)} = \left\{ u^{\circ}M^{\circ}(\xi) \left[\underline{f}(x^{\prime}\nabla^{\xi}) - \underline{f}(x^{\prime}\nabla)\right] \right\} \xi$$

since,

(10)
$$\frac{\partial x}{\partial \underline{f}(x'p)} = \frac{\partial u}{\partial f(u'p)} \cdot u^o = u^o (\underline{f}(u+i'p) - \underline{f}(\iota'p))$$

and dropping the bar and writing

$$(11) \qquad \qquad W(\mathcal{E}) = n_o \, W_i(\mathcal{E})$$

(10")
$$\frac{\partial x}{\partial f(x, \Delta)} = \int_{\infty}^{\infty} M(\varepsilon) \left[f(x, \Delta - \varepsilon) - f(x, \Delta) \right] d\varepsilon$$

we obtain the Landau differential-integral equation (5) and need an estimate of \mathbf{N}_{o} . In the first place

$$(12) \qquad \qquad \mathbf{\xi} = \frac{\mathbf{e^4}}{\mathsf{E_b b^2}}$$

where **b** is the "impact parameter" of the collision. The electrons that will "collide" with the incoming electron will lie within the range b_i and b_2 corresponding to max and min energy loss per collision. For an electron traveling unit distance the colliding electrons will fill volume $\pi(b_i^1 - b_i^2) \cdot 1$ or

(13)
$$\frac{\text{Tre}^4}{\text{E}_0} \left(\frac{1}{\xi_1} - \frac{1}{\xi_2} \right), \quad (\text{cm}^3/\text{cm.path})$$

The density of "fixed" electrons is

$$\frac{Ng \Sigma Z}{\Sigma A}, \qquad \left(\frac{\text{electrons}}{Cm^3}\right)$$

so that

(15)
$$n_0 = \frac{\pi e^4 N_S \sum Z}{E_1 \sum A} \left(\frac{\xi_2 - \xi_1}{\xi_2 \xi_1} \right), \quad \left(\frac{\text{electrons}}{G_{11}, \text{path}} \right)$$

or

$$(16) W(x) = \frac{a}{x^2}$$

where,

(17)
$$a = \frac{\pi e^4 N_5 \Sigma Z}{E_a \Sigma A}.$$

The physical argument involves two reasonable assumptions:

- A. it makes no physical sense to estimate of on closer than a difference quotient involving a single collision.
- B. $x = \frac{n}{n_o}$ is a sufficiently good estimate of the depth reached in n collisions so that we can equate

(18)
$$\frac{\partial f}{\partial x} = n_o \left(f(n+1, \Delta) - f(n, \Delta) \right)$$

The preceding discussion shows that ξ in $W(\xi)$ stands strictly for the energy loss per impact and $\frac{W(\xi)}{N_o} = W_i(\xi)$ is the probability density for this loss.

Landau's Approximating Solution of His Differential Integral Equation.

Landau's approximating solution of his differential-integral equation was reached by the use of Laplace transforms. Let

(19)
$$\phi(x,p) = \int_{a}^{\infty} f(x, \Delta) e^{-p\Delta} d\Delta$$

Then, by the inversion theorem,

(20)
$$f(x,\Delta) = \frac{1}{2\pi i} \int_{-i\phi+\sigma}^{i\phi+\sigma} \phi(x,p) dp$$

Taking the Laplace transform of equation (5) gives

(21)
$$\frac{\partial x}{\partial \phi(x,b)} = -\phi(x,b) \int_{0}^{\infty} w(\varepsilon) (1-e^{-b\varepsilon}) d\varepsilon$$

because,

$$e^{-p\epsilon} \phi(x_{j}p) = \int_{0}^{\infty} e^{-p\Delta} f(x_{j}\Delta - \epsilon) d\Delta$$

$$= \int_{0}^{\infty} e^{-p(\Delta' + \epsilon)} f(x_{j}\Delta') d\Delta'$$

$$= e^{-p\epsilon} \int_{0}^{\infty} e^{-p\Delta'} f(x_{j}\Delta') d\Delta'$$

Equation (21) is now an ordinary differential equation in x satisfying the initial condition,

$$f(0,\Delta) = S(\Delta)$$
 or $\phi(0,p) = 1$

The solution is therefore

The solution is therefore
$$w(\varepsilon)(1-e^{-\beta\varepsilon})d\varepsilon$$
(22) $\phi(x,y) = e^{-\lambda \int_{0}^{\infty} w(\varepsilon)(1-e^{-\beta\varepsilon})d\varepsilon}$

or, more clearly

where,

(23)
$$C_{i}(p) = \int_{0}^{\infty} W_{i}(\epsilon) e^{-p\epsilon} d\epsilon$$

=. moment generating function for the probability density W₁(£) for energy loss per collision.

It then follows that,

(24)
$$f(x, \Delta) = \frac{1}{2\pi i} \int_{-i\omega+\tau}^{+i\omega+\tau} e^{+i\omega+\tau} dt$$

This Landau's general expression for the distribution function 🕏 in terms of the function W(1) where W(2) d2 is the number of collisions per unit path length with energy loss between & and £+48. To proceed further, Landau, in effect, takes:

(16)
$$W(\varepsilon) = \frac{\alpha}{\varepsilon^{2}}$$

$$\alpha = \frac{\pi e^{4} N \rho \Sigma Z}{E_{o} \Sigma A}$$

$$\varepsilon_{1} = \frac{(1 - \rho^{2}) I^{2}}{4E_{o}} e^{\beta^{2}}$$

$$\beta = \frac{V}{c}, I = I_{o} Z$$

$$\varepsilon_{2} = \infty, I_{o} = 13.5 \text{ eV}$$

To see this, we follow his steps where he approximates the integral

(25)
$$\int_{0}^{\infty} W(\varepsilon) \left(1 - e^{-t\varepsilon}\right) d\varepsilon = \int_{0}^{\varepsilon} \sum_{k=0}^{\infty} w(\varepsilon) d\varepsilon + \int_{0}^{\infty} w(\varepsilon) \left(1 - e^{-t\varepsilon}\right) d\varepsilon$$

where $\xi_1 < \xi^0 < \xi_2$. To evaluate the first integral on the right hand side he refers to a result from Livingston and Bethe, Rev. Mod. Phys. 9 245 (1937), i.e.,

(26)
$$\int_{-\infty}^{\infty} z w(z) dz = a \ln \frac{z^{\bullet}}{z_{i}}, \quad \ln z^{\bullet} = \ln \frac{(1-\beta^{2}) J^{2}}{4 E_{\bullet}} + \beta^{2}$$

We notice that if we take $W(\xi) = \frac{q}{\xi}$ in the region $\xi_1 < \xi < \xi^{\circ}$ $\int_{\xi_1}^{\xi_2} \xi w(\xi) d\xi = a \ln \frac{\xi^{\circ}}{\xi_1}$

and that in effect Landau uses the law

over the interval \mathcal{I}_i to $\mathcal{I}_{2,2} \Rightarrow$. In addition he makes the approximation

in the region, $\xi, \xi \xi \xi$. This will work for sufficiently small ξ .

Integrating the second term on the right by parts

$$\frac{1}{r} \int_{\xi_{0}}^{\infty} \frac{1 - e^{-r\xi}}{\xi^{2}} = \frac{1}{r^{2}} (1 - e^{-r\xi^{0}}) + \int_{\xi_{0}}^{\infty} \frac{e^{-r\xi}}{\xi} d\xi$$

Substituting 2=42 and noting that again that

gives
$$\frac{1}{p} \int_{\xi^{0}}^{1-e^{-p\zeta}} d\xi = 1 + \int_{\xi^{0}}^{\infty} \frac{e^{-\frac{1}{2}} dz}{z}$$

$$= 1 + \int_{\xi^{0}}^{\infty} \frac{dz}{z} + \int_{0}^{\infty} \frac{e^{-\frac{1}{2}}}{z} dz + \int_{0}^{\infty} \frac{e^{-\frac{1}{2}}}{z} dz$$

where

$$\int_{0}^{1} \frac{e^{-\frac{7}{2}} + \int_{0}^{\infty} \frac{e^{-\frac{7}{2}}}{2} = -C$$

(Ryshik-Gradstein: "Tables of Series, Products, and Integrals," VEB Deutscher verlag der Wiss, Berlin, 1957 p.306)

where

Hence

(27)
$$\int_{\xi^*}^{\infty} \frac{1 - e^{-\gamma \epsilon}}{\epsilon^*} d\epsilon = \beta \left(1 - C - \ln \beta \epsilon^* \right)$$

and

(28)
$$\int_{0}^{\infty} w(\xi) (1 - e^{-t\xi}) \stackrel{!}{=} pa (1 - C - ln p \xi^{\bullet}) - pa ln \frac{\xi}{\xi^{\bullet}}$$

$$\stackrel{!}{=} pa (1 - C - ln p \xi_{i})$$

We can now write,

$$f(x, \Delta) = \frac{1}{2\pi i} \int_{-i\Delta+\sigma}^{+i\Delta+\sigma} \left[\Delta - ax(1-C-4n+\epsilon_i) \right] d\epsilon$$

If we write

(29)
$$\begin{cases} \xi = ax, & N = p \\ \lambda = \frac{\Delta}{\xi} - k_1 \frac{\xi}{\xi} + C - 1 \end{cases}$$

Then

$$(30) f(x,\Delta) = \frac{\phi(\lambda)}{5}$$

where

(31)
$$\phi(\lambda) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{iknu + \lambda u}$$

is Landau's "universal function, carefully studied and calculated by Börsch-Supan.

Physically it is seen that Landau makes two assumptions

A. The distribution
$$W(\xi) = \begin{cases} 4/\xi^2, & \xi_1 < \xi < \xi_2 \\ 0, & \text{else where} \end{cases}$$
where $\xi_1 = \frac{(1-\beta^2)\tilde{J}^2}{4\xi_0} \cdot e^{\beta^2}$

B. We don't have to estimate $\mathcal{E}_{\mathbf{k}}$ because the contribution to the energy loss is negligibly increased by taking $\mathcal{E}_{\mathbf{k}} = \mathbf{e}$ instead of \mathcal{E}_{max} .

An Alternative Approach - The Method of Moments.

After critically examining Landau's solution, several alternatives to obtaining a tractable solution suggest themselves. In the first place, if $W_1(\xi)$ is the probability density for the energy loss in a single collision and we take $\times n_0$ to be the number of collisions in going a distance x_0 . Then the moment generating function $\phi(x_0, y_0)$ is given by

(32)
$$d(x, y) = [c, (y)]^{n,x} = e^{n,x} ln [1 - (1 - c, y)]$$

where,

(33)
$$C_{1}(p) = \int_{0}^{\infty} w_{1}(z) e^{-\frac{1}{2}} dz$$

but

Or we get

Or we get
$$(33') \qquad \varphi(x,p) = e^{-h \cdot x} \left\{ \sum_{m=1}^{\infty} \frac{\left[1 - C_{n}(x)\right]^{m}}{m} \right\}$$

to compare with the Landau solution via the differential-integral equation

To compare the two in another way, e.g. in their estimate of the first two moments, notice, that

$$C_{1}(p) = \int_{0}^{\infty} W_{1}(\epsilon) e^{-p\epsilon} d\epsilon$$

$$= \int_{0}^{\infty} W_{1}(\epsilon) \sum_{n=1}^{\infty} \frac{(-p\epsilon)^{n}}{m!} d\epsilon$$

$$= \sum_{n=1}^{\infty} \frac{\mu_{n}}{n!} (-p)^{n}$$

where

or

hence the name moment generating function.

1f

then

$$\frac{\partial b}{\partial \phi(x,b)}\Big|_{b=0} = -A$$

$$\frac{\partial^2 d(x,p)}{\partial b^2} \bigg|_{b=0} = B , ek.$$

but

$$\frac{\partial \phi(x,p)}{\partial \phi} = n_{0}x \left[1 - \mu_{1}p + \frac{\mu_{2}}{2}p^{2}\right] - (-\mu_{1} + \mu_{2}p)$$

$$\frac{\partial \phi(x, p)}{\partial p}\Big|_{p=0} = -A = -n_0 \times \mu_1 = -n_0 \times \overline{\epsilon}$$

$$\frac{\partial^{2}\phi(x,p)}{\partial p^{2}} = n_{0}x \left(n_{0}x-1\right) \left[1-\mu_{1}p + \frac{\mu_{2}}{2}p^{2}\right]^{n_{0}x-2} \left(-\mu_{1}+\mu_{0}p\right)^{2}$$

$$+ n_{0}x \left[1-\mu_{1}p + \frac{\mu_{2}}{2}p^{2}\right]^{n_{0}x-1} \left(\mu_{0}p\right)^{2}$$

5

$$\frac{\partial f^{2}}{\partial f^{2}}\Big|_{b=0} = B = 0.x (N.x-1) \mu_{1}^{2} + N.x \mu_{2}$$

and

$$B-A^2 = h_0 \times (\mu_2 - \mu_1^2) = h_0 \times \sigma^2$$

li, on the other hand,

$$\phi(x,p) = e^{-Nox(1-C_1(p_1))} = 1 - Ap + \frac{B}{2}p^2 + ...$$

$$= e^{-Nox(\mu_1 p - \frac{\mu_2 p^2}{2})}$$

$$= 1 - Nox(\mu_1 p - \frac{M_1 p^2}{2}) + \frac{1}{2}(Nox)^2(\mu_1 p - \frac{M_2 p^2}{2})^2$$

$$= 1 - Nox\mu_1 p + \frac{1}{2}[Nox\mu_2 + (Nox)^2\mu_1^2]p^2 + ...$$

so that

then

The implication of this result is that the variance of \(\sum_{\text{o}} \) computed by the Landau differential-integral equation will be too large by a factor

$$\frac{\mu_z}{\mu_z - \mu_z^2} = \frac{1}{1 - \frac{\mu_z^2}{\mu_z}}$$

But

$$\mu_{1} = \frac{\xi_{1}\xi_{2}}{\xi_{2}-\xi_{1}} \int_{\xi_{1}}^{\xi_{2}} \frac{d\xi}{\xi} = \frac{\xi_{1}}{1-\frac{\xi_{1}/\xi_{2}}} \ln \frac{\xi_{2}/\xi_{1}}{\xi_{1}}$$

$$\mu_{2} = \frac{\xi_{1}\xi_{2}}{\xi_{2}-\xi_{1}} \int_{\xi_{1}}^{\xi_{2}} d\xi = \frac{\xi_{1}\xi_{2}}{\xi_{1}\xi_{2}} = \frac{\xi_{1}^{2}/\xi_{2}}{\xi_{1}/\xi_{2}}$$

Hence,
$$\frac{1}{1 - \frac{M^2}{\mu_2}} = \frac{1}{1 - \frac{\xi_1 \xi_2 \left(\ln \xi y_{\epsilon_1} \right)^2}{\left(\xi_1 - \xi_1 \right)^2}} = \frac{1}{1 - \frac{\mu \left(\ln \mu \right)^2}{\left(y_{\epsilon_1} \right)^2}}$$

where

$$M = \frac{2E_0}{I} = \frac{2E_0}{I} = \frac{2\times 10^6}{10} = 2\times 10^5$$
. =. in a case of interest,

hence,

$$\frac{1}{1 - \frac{M^2}{\mu_2}} = \frac{1}{1 - \frac{2 \cdot 10^{5} \cdot (4 \cdot M)^2}{(2 \cdot 10^{5})^{\frac{3}{2}}}} = 1 + 8 \times 10^{-5}$$

Also,

It would seem, as might be expected on the grounds of the reasonableness of both models, that the numerical error is small. Nevertheless, the expression based on random walk, i.e.,

where

(33)
$$C_{i}(p) = \int_{0}^{\infty} W_{i}(\varepsilon) e^{-p\varepsilon} d\varepsilon$$

where

 $W_{i}(\xi)$.=. distribution of ξ , energy less per collision

seems conceptually simpler and may lead to a more tractable inversion to obtain $f(x,\Delta)$. This inversion is being worked on but has so far resisted all attempts.

On the satisfactory solution of the inversion problem rests the easy calculation of straggling due to windows in series.

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